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The automated xpdf beamline at diamond light source

Philip Anthony Chater¹, Dean Keeble¹, Michael Wharmby¹, Timothy Spain¹, Jacob Filik¹, Heribert Wilhelm¹

**Diamond Light Source, Didcot, United Kingdom

E-mail: philip.chater@diamond.ac.uk

XPDF is the new, independent side-station to the Extreme Conditions beamline I15 at Diamond Light Source. It is committed to the fast and reliable production of pair distribution function (PDF) data. Here we present an overview of the XPDF beamline hardware, and the software which makes automation possible.

The beamline optics deliver X-ray energies of 40, 65 or 76 keV with a tunable bandwidth, allowing experiments to be optimised for rapid data collection (high bandwidth) or high resolution (low bandwidth). Two area detectors can be independently positioned at different sample-to-detector distances allowing for simultaneous PDF and higher resolution Bragg data collections.

Alongside optimised hardware, significant effort has been put into software to produce a user-friendly, automated beamline. Integrated data collection and analysis software has been developed which will perform automatic data processing to deliver real-time Bragg, total scattering and PDF data. 2-D scattering data from an area detector can be corrected, integrated to 1-D and processed to X-ray PDFs, all from within a single interface. The PDF processing pipeline and examples of typical experiments performed on the XPDF beamline will be presented. The new PDF processing software is freely available as part of the DAWN software package [1].

[1] Basham M., Filik J., Wharmby M. T., Chang P. C. Y., El Kassaby B., Gerring M., Aishima J., Levik K., Pulford B. C. A., Sikharulidze I., Sneddon D., Webber M., Dhesi S. S., Maccherozzi F., Svensson O., Brockhauser S., Náray G. & Ashton A. W. (2015). J. Synchrotron Rad., 22, 853.

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